Applied Mathematics and Computation 281 (2016) 233–242

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Distance-based topological indices of the tree-like polyphenyl systems☆

Ailian Chen, Xianzhu Xiong, Fenggen Lin*

College of Mathematics and Computer Science, Fuzhou University, Fuzhou, Fujian 350116, China

ARTICLE INFO

MSC:
05C12
05C78
05C05

Keywords:
Wiener index
Polyphenyl chain
Topological index
Degree distance
Szeged index

ABSTRACT

Topological indices based on the distances between vertices(atoms) of a molecular graph are widely used for characterizing molecular graphs and their fragments, establishing relationships between structures and properties of molecules, predicting biological activity of chemical compounds, and making other chemical applications. Polyphenyls are a kind of macrocyclic aromatic hydrocarbons and their derivatives are very important organic chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc. In this paper we investigate the relationships between the Wiener index and other distance-based topological indices in the tree-like polyphenyl systems and obtain some exactly formulae on the relationships.

1. Introduction

Topological indices based on the distances between vertices of a graph are widely used for characterizing molecular graphs and their fragments, establishing relationships between structures and properties of molecules, predicting biological activity of chemical compounds, and making other chemical applications[8,23,24,39,61]. Their history goes back to 1947, when Harold Wiener [63] used the distances in the molecular graphs of alkanes to calculate their boiling points. This pioneering research led to the topological index named Wiener index that became one of the most popular molecular structure descriptors. It found numerous applications for QSPR and was applied elsewhere, say in crystallography, communication theory, facility location, etc., cf. [4]. Other important distance-based topological indices which are introduced later will be defined in Section 2, which include the edge-Wiener index [48,59], the vertex-Szeged index [20,41], the edge-Szeged index [21], the PI index [42] etc. For the state of the art on the distance in molecular graphs see the recent books [23,24]. For the role of distance-sum-based molecular descriptors in a drug discovery process we refer to [53] and the references therein.

Polyphenyls are a kind of macrocyclic aromatic hydrocarbons and their derivatives are very important organic chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc, see [18,50,60] and the references therein. Many years ago, a series of linear and branched polyphenyls and their derivatives were synthesized and some physical properties were discussed [32,33,54–57]. Gutman and Dömötör [22] showed that the values which the Wiener indices of isomeric polyphenyls may assume are all congruent module 36. In [3,16,28] the authors determine the polyphenyl chains with extremal Wiener indices, edge-Wiener indices and degree distances among all the polyphenyl chains with h hexagons,

☆ Supported by the National Natural Science Foundation of China (nos. 11301084, 11301085 and 11401102).
* Corresponding author. Tel.: +86 18950468419.
E-mail addresses: elian1425@sina.com (A. Chen), xiongxianzhu2001@sina.com (X. Xiong), linfenggen@163.com (F. Lin).

http://dx.doi.org/10.1016/j.amc.2016.01.057
0096-3003/

respectively. In [9] the author give an explicit formulae for computing the Wiener indices of th polyphenyl chains. For more recent results on polyphenyl systems we refer to see [2,10,28,30,31,65,66].

In this paper we investigate the relationships between the Wiener index and other distance-based topological indices in the tree-like polyphenyl systems and obtain some exactly formulae on the relationships. Our results reduce the problems on the distance-based indices investigated in this paper to those on the Wiener index of the tree-like polyphenyl systems, which make the former easier.

2. Preliminaries

In this paper, all graphs are finite, undirected, simple connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The line graph $L(G)$ of G, is the graph with the edge set $E(G)$ as its vertex set, in which two vertices are joined by an edge if they have a common vertex in G. $deg_G(u)$ denotes the degree of the vertex u in G. Under distance $d_G(u, v)$ between vertices $u, v \in V(G)$ we mean the standard distance of the graph G, i.e., the number of edges on a shortest path connecting u and v in G. The distance of a vertex $v \in V(G)$, $D_G(v)$, is the sum of distances between v and all other vertices of G. Under distance $d_G(e, f)$ between edges $e, f \in E(G)$ we mean the standard distance of e and f in $L(G)$. The distance of an edge $e \in E(G)$, denoted by $D_G(e)$, is the sum of distances between e and all other edges of G.

Definition. The *Wiener index* of a graph G is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in G [63]:

$$W(G) = \sum_{\{u,v\}\subset V(G)} d_G(u, v) = \frac{1}{2} \sum_{v\in V(G)} D_G(v).$$

Edge versions of the Wiener index based on the distances between all pairs of edges in a connected graph G were introduced in 2009 [36].

Definition. The *edge-Wiener index*of a graph G is denoted by $W_e(G)$ and defined as

$$W_e(G) = \sum_{\{e,f\}\subset E(G)} d_G(e, f).$$

Note that the edge-Wiener index of G is nothing but the Wiener index of the line graph $L(G)$ of G, that is, $W_e(G) = W(L(G))$. The concept of line graph has found various applications in chemical research [27,61]. For the hitherto obtained results on the edge-Wiener index, we refer to see the review [37] and the references therein.

As a vertex-degree-weighted version of Wiener index, the degree distance of a graph G is independently proposed by Dobrynin and Kochetova [14] and Gutman [20].

Definition. The *degree distance* of a graph G is denoted by $DD(G)$ and defined as

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} [deg_G(u) + deg_G(v)]d_G(u, v) = \sum_{v\in V(G)} deg_G(v)D_G(v).$$

Let $e = (u, v) \in E(G)$, denoted by $n_u(e)$ the number of vertices of G whose distance to u is smaller than the distance to v and $m_u(e)$ is the number of edges of G whose distance to u is smaller than the distance to v, respectively.

Motivated by the following property of the Wiener index of a tree T [63]:

$$W(T) = \sum_{e=(u,v)\in E(T)} n_u(e)n_v(e),$$

Gutman [19] introduced the *Szeged index* of a graph G as

$$S_z(G) = \sum_{e=(u,v)\in E(G)} n_u(e)n_v(e).$$

Evidently, $Sz(T) = W(T)$ holds for any tree T.

The other distance-based topological indices, such as *edge-Szeged index* $S_e(G)$ [21], *PI index* $PI(G)$ [42], *Gutman index* $Gut(G)$ [20], *Wiener polarity* index $W_P(G)$ [63] and *generalized terminal Wiener index* $TW_r(G)$ [34] of G are defined as follows:

$$S_{z_e}(G) = \sum_{e=(u,v)\in E(G)} m_u(e)m_v(e),$$

$$PI(G) = \sum_{e=(u,v)\in E(G)} [m_u(e) + m_v(e)],$$

$$Gut(G) = \sum_{\{u,v\}\subset V(G)} deg_G(u)deg_G(v)d_G(u, v),$$

$$W_p(G) = |\{\{u, v\} \subseteq V(G)|d_G(u, v) = 3\}|,$$

$$TW_r(G) = \sum_{\substack{\{u,v\}\subset V(G),\\ deg_G(u)=deg_G(v)=r}} d_G(u, v).$$